N-Benzyl O-propyl thiocarbamate

Inchi: InChI=1S/C11H15NOS/c1-2-8-13-11(14)12-9-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,
InchiKey: KTOIPILWYSRXQY-UHFFFAOYSA-N
Formula: C11H15NOS
SMILES: CCCOC(S)=NCc1ccccc1
Mol. weight [g/mol]: 209.31

Physical Properties

Property code	Value	Unit	Source
hf	-55.15	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.899		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2868.00		NIST Webbook
ripol	2868.00		NIST Webbook
tb	639.60	K	Joback Method
tc	879.51	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R440023&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature